Table 47. SGI/Cray T3D Timings for *SUPERMOLECULE 1.08*.[a]

Benchmark	Basis	# Proc.'s	Heterogen.	Wall Time
Ethylene	6-311++G**[b]	64	No	67
		128	No	70
Imidazole	6-311++G*[c]	64	No	203
		128	No	133
		256	No	133
18-crown-6	3-21G[d]	64	No	270
		128	No	218
		256	No	242
		512	No	271
	6-31G**	128	No	1298
		256	No	1080
		512	No	914
		1024	No	977
		256	Yes	752
		512	Yes	583
	aug-cc-pVDZ	256	No	5621
		512	No	4044
		1024	No	3553
		256	Yes	4128
		512	Yes	2534
		1024	Yes	2035

[a]All times are in seconds. All runs are single point direct Hartree-Fock calculations. Heterogenoeus runs split the calculation across the C90 and the T3D. Calculations were run by Dr. Martin Feyereisen of Cray Research, Inc.

[b]Total time on a single C90 processor = 20 sec.

[c]Total time on a single C90 processor = 679 sec.

[d]Total time on a single C90 processor = 1224 sec.